

Modeling the Effects of In-Cylinder Flows on HSDI Diesel Engine Performance and Emissions

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ABSTRACT

In the present work the three-dimensional KIVA CFD code was used to simulate the combustion process in a HSDI diesel engine. State-of-the-art models, including the KH-RT spray breakup model, the RNG $k-\varepsilon$ turbulence model, and a n-heptane reduced chemistry including reduced GRI NOx mechanism were used. The performances of two combustion models, KIVA-CHEMKIN and GAMUT (KIVA-CHEMKIN-G), coupled with 2-step and multi-step phenomenological soot models were compared. The numerical results were compared with available experimental data obtained from an optically accessible HSDI engine and good agreement was obtained. To assess the effects of the in-cylinder flow field on combustion and emissions, off-centered swirl flows were also considered. In these studies, the swirl center was initialized at different positions in the chamber for different cases to simulate the effects of different intake flow arrangements. To aid the comparisons, the angular momentum referred to the swirl center was kept constant in each case. Numerical results of off-centered swirl cases were compared with the centered swirl case, as well as with available experimental images obtained using laser induced fluorescence (LIF), laser induced incandescence (LII), and particle image velocimetry (PIV). Eccentric phenomena observed in the experiments were well predicted by the present method. The off-centered swirl was found to have higher turbulence intensities and effective diffusivities, which enhance the mixing process. Soot formation is strongly correlated with the turbulent viscosity. Off-centered swirl flow results in an asymmetric distribution of turbulent viscosity and consequently an asymmetric distribution of soot emissions. Analysis of the mass distributions of temperature showed that the resulting mixture is a little more homogeneous with larger off-centered swirl flows, which leads to a slight reduction in NOx emissions. The off-centered swirl delays the formation of acetylene, which changes the phasing of soot formation.

INTRODUCTION

Impending worldwide energy resource crises and pressure from environmental regulations motivate the development of new engines with high thermal efficiency and low pollutant emissions. Direct injection (DI) diesel engines have a high potential for reduction of CO₂ emissions. Good reliability and affordable cost make them very attractive for today's market. However, PM and NOx emissions from diesel engines need to be simultaneously reduced to meet current and future strict emission regulations.

Engine pollutant emissions are directly determined by the in-cylinder mixing and consequent combustion processes. High temperature is a condition that promotes the formation of NOx and soot. Thus, many techniques are being explored to reduce the local temperature in-cylinder, which are labeled "low temperature combustion" (e.g., Fang et al. [1]). The highest temperature occurs in regions with nearly stoichiometric mixtures. Therefore, a cool, homogeneous, lean mixture is targeted for low emissions operation. Swirl can enhance mixing processes and may lead to a more homogeneous mixture. EGR can reduce NOx emissions by diluting the fresh mixture, because reduced oxygen concentration helps minimize thermal NO formation. If the EGR is cooled, the in-cylinder temperature can be reduced. Many optimization studies have also focused on piston bowl design and spray targeting. The ultimate goal is to provide a homogeneous lean mixture without rich regions that could lead to soot formation.

In-cylinder flow control is one of the key methods available to control the combustion process in diesel engines. However, except for the fuel injection process, there is little that can be done to the in-cylinder flows after intake valve closure (IVC). Therefore, a good flow pattern should be prepared before IVC, which can be characterized by optimized swirl and tumble. Swirl is the only large scale motion which is retained during the compression stroke. An appropriate swirl can enhance

the mixing process, and consequently increase the combustion efficiency and reduce pollutant emissions. Understanding how to prepare such swirl is of great importance. In the present paper, centered and off-centered swirl flow patterns are investigated using multi-dimensional CFD analysis. The effects of flow eccentricity on combustion performance are compared with centered swirl results since it is often assumed that the in-cylinder flows are symmetric with respect to the axis of the cylinder.

The CHEMKIN-II chemistry solver package was implemented into the KIVA-3V code by Kong et al. [2]. CHEMKIN can deal with arbitrarily complicated chemical reaction mechanisms, with which the processes of ignition/extinction and pollutant formation can be described in a very detailed way. Recently, a G-equation level-set model for describing turbulent flame propagation has been developed and implemented into the KIVA-3V code by Tan and Reitz [3]. This G-equation-based model has been used to simulate both SI [3-8] and diesel engines [5, 9-11], and a dual-fuel CI engine [9]. Encouraging results have been obtained using the KIVA-CHEMKIN-G model that has been called the GAMUT (G-equation for All Mixtures, a Universal Turbulent) combustion model.

In this study, the performance of KIVA-CHEMKIN and the GAMUT combustion model were examined on a HSDI diesel engine by comparing simulation results with available experimental results. A 2-step soot model [12] and a multi-step phenomenological soot model [13] were employed. Their performances coupled with the different combustion models were compared and analyzed. In addition, the effects of off-centered swirl flow on engine performance and pollutant emissions were studied.

OPTICAL ENGINE AND OPERATING CONDITIONS

The engine simulated in the present work is a state-of-the-art, small-size class, optically accessible, HSDI diesel engine, shown in Fig.1. It is based on a four-cylinder production engine, and has a four valve cylinder head. The injector is located vertically at the center of the fire deck. The piston bowl is ω -shaped (c.f., Fig.3). A common-rail injection system is used with the engine. The piezo-actuated injector has a nozzle tip with six equally-distributed, hydro-eroded holes. Three quartz glass windows and a quartz piston bowl are installed on the fourth cylinder for laser access. Optical distortions were reduced by means of a spherical surface at the bottom side of the piston bowl. The whole bowl volume and part of the squish zone are visible through the piston bowl window. Several measurement techniques were applied to the engine, including laser induced fluorescence (LIF), laser induced incandescence (LII), particle image velocimetry (PIV), fast gas sampling valve, etc. Detailed descriptions of the experimental setup can be found in [14-16].

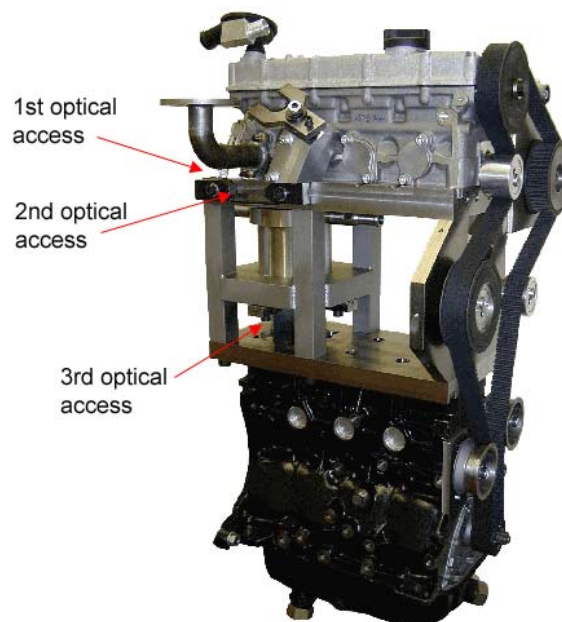


Figure 1. optical HSDI diesel engine

Table 1 Specifications and operating conditions of the HSDI engine [14-16].

Type of Engine	HSDI diesel, Optically-accessible
Piston bowl	ω -shaped
Bore x Stroke	79.5 x 95.5 [mm]
Displacement	474 [cm ³]
Simulated Compression Ratio	16.5
Engine Speed	1500 [rev/min]
IVC	-104 [° ATDC]
EVO	131 [° ATDC]
EGR	25%
Swirl Ratio	1.75
Load	3 bar/5 bar IMEP
Fuel Injector (FEV CORA II)	Piezo-actuated, 6 holes (uniformly distributed)
Pilot SOI/DOI	-30/~2.5 [° ATDC]
Main SOI/DOI	1/~4.0 [° ATDC]
Spray angle	150 °
Injection Pressure	800/1000 [Bar]

The specifications and operating conditions of the engine are summarized in Table 1. The engine is optimized to achieve the same power output on the basis of similar pressure traces and similar engine emissions as the real four-cylinder engine. In this way, the optically accessible engine has the same thermodynamic conditions during the combustion process as the real engine. The measurements are thus considered to be representative of conventional diesel engine combustion. Figure 2 shows the injection rate profiles with injection pressure of 800 and 1000 bar, respectively. A multiple injection strategy is employed where the early injection occurs at around -30 degrees ATDC and prepares a partially premixed mixture for the main combustion process.

after the main injection at around 1 degree ATDC. The pilot and main injection duration (DOI) are 2.5 and 4 degrees, respectively.

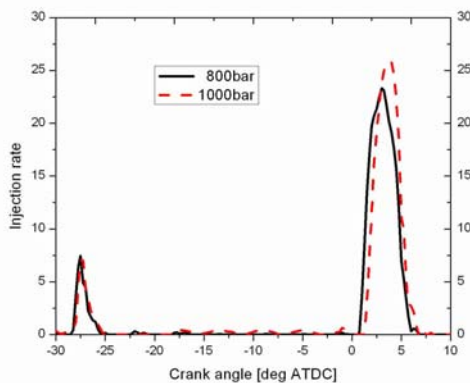


Figure 2. injection rate profiles

MODELING METHODOLOGY

In the present work, the ERC version of the KIVA-3V Release 2 code was used to simulate the combustion processes in the HSDI diesel engine. Two combustion models were considered: the KIVA-CHEMKIN model [2], and the GAMUT combustion model [11]. The KIVA-CHEMKIN model assumes that each computational cell is a perfectly-stirred reactor (PSR). Coupled with an appropriate reaction mechanism, the thermo-chemical state of each cell is then computed using the CHEMKIN package. The GAMUT combustion model is a hybrid auto-ignition and flame propagation model. As in the KIVA-CHEMKIN model, the auto-ignition process is modeled using CHEMKIN. However, the flame front propagation is considered and it is represented by an iso-scale surface (usually the scalar $G=0$), and the flame propagation process is then modeled by tracking the location of this surface. The transport equation of the iso-G surface is written as

$$\rho \frac{\partial G}{\partial t} + \rho \vec{U} \cdot \nabla G = \rho s_L |\nabla G| \quad (1)$$

and it is solved using a level-set method [17]. The second term on the left-hand side is the convective term. The term on the right-hand side is the propagation term which accounts for the chemical properties of the mixture. Stretch effects on the flame are reflected in the curvature of the G surface. Therefore, the turbulence-combustion interactions are described by the G -equation.

Peters [18] modeled the G -equation for the corrugated flamelet regime and the thin reaction zone regime in the framework of the RANS turbulence model. Tan [3] developed the G -equation for engine simulation and demonstrated that it could be used for both premixed and non-premixed combustion situations. Considering the moving meshes used in engine codes, the modeled equations for the Favre-averaged G are written as

$$\frac{\partial \tilde{G}}{\partial t} + (\tilde{U}_{bf} - \tilde{U}_{vertex}) \cdot \nabla \tilde{G} = \frac{\bar{\rho}_u}{\bar{\rho}} s_T^0 |\nabla \tilde{G}| - D_T \tilde{\kappa}_M |\nabla \tilde{G}| \quad (2)$$

The computational domain is separated into three parts: the region ahead of the flame front (unburned region, $G < 0$), on the flame front region ($G = 0$), and the regions behind the flame front (burned region, $G > 0$). The cells ahead and behind the flame are treated as PSRs, i.e., the KIVA-CHEMKIN model is used to compute their thermo-chemical states. In this way, auto-ignition processes are predicted using CHEMKIN, and computational cells with temperatures greater than 1100K are regarded as ignition sites. As soon as an ignition kernel is formed, the flame propagation model is activated. If the characteristic length of the ignition kernel region is larger than the averaged turbulent integral length scale, a G surface is initialized. The cells on the flame front are assumed to be in chemical equilibrium, that is complete combustion is assumed to occur across the flame. Therefore, the chemical equilibrium assumption can lead to higher heat release and temperatures, fewer hydrocarbon species, and more reaction products than the results obtained using the PSR assumption in the KIVA-CHEMKIN model. The change of composition in a computational cell containing the flame front is given as

$$\frac{dY_i}{dt} = (Y_i^u - Y_i^b) \frac{A}{V} s_T^0 \quad (3)$$

where A and V are the flame surface area and volume of the computational cell, respectively. Y_i is the mass fraction of the i -th species. The superscripts "u" and "b" refer to the values in the unburned and burned regions, respectively.

The GAMUT combustion model has been used extensively to simulate combustion in spark-ignited gasoline engines, in which the combustion process is a typical premixed combustion [3-8]. It has also successfully been applied to simulate diesel/natural-gas dual-fuel CI engine [9] and conventional diesel engines [5, 9-11]. For dual-fuel CI engines, the natural-gas is premixed with air before the diesel fuel is ignited. Therefore, it is necessary to account for the flame propagation phenomena in numerical simulations. Previous study [9] has proven that the GAMUT combustion model gives better predictions than the KIVA-CHEMKIN model for the dual-fuel CI engine. The diesel engine simulated in the present work features multiple injections and the fuel injected during the pilot injection mixes with the air before the main injection. If the resulting mixture is rich enough, a flame created by the auto-ignition of the diesel fuel may propagate into partially premixed diesel/air mixtures. Therefore, it is of much interest to explore the performance of the GAMUT combustion model for modeling multiple injections in diesel engines.

Both the KIVA-CHEMKIN and GAMUT combustion models consider detailed chemistry. In the present work, the ERC reduced n-heptane mechanism with 34 species

and 74 reactions was used [19]. Other models include the ERC crevice model, KH-RT spray breakup model, and the RNG $k-\epsilon$ turbulence model. A NO_x formation mechanism, which was adapted from the GRI methane/air combustion mechanism, has been included in the reduced ERC kinetics mechanism. Two different soot models were employed in the present computations: Hiroyasu's 2-step soot model [12, 20] and a multi-step phenomenological soot model [13]. Acetylene is included in the ERC n-heptane mechanism, and both soot models take acetylene as the growth/soot inception species instead of fuel vapor. The fuel pyrolysis reactions and acetylene oxidation proposed by Tao et al. [13] were removed, because they are included in the chemistry mechanism. In the 2-step soot model, two empirical expressions for soot formation and soot oxidation are used. The net soot production rate is determined from

$$\frac{dM_s}{dt} = \frac{dM_{sf}}{dt} - \frac{dM_{so}}{dt}, \quad (4)$$

where the soot formation rate is given by

$$\dot{M}_{sf} = \frac{dM_{sf}}{dt} = A_{sf} \rho_{C_2H_2} p^n \exp\left(-\frac{E_{sf}}{RT}\right), \quad (5)$$

where $\rho_{C_2H_2}$ is the partial density of acetylene; p is the pressure; T is the temperature; E_{sf} is the activation energy (12500 cal/mol [12]); A_{sf} is the Arrhenius pre-exponential factor normally set to 40; and the exponential factor for pressure, n is set to 0.5 [12].

The soot oxidation rate is determined using the Nagle and Strickland-Constable model [21], and is calculated as

$$\frac{dM_{so}}{dt} = \frac{6MW_c}{\rho_s D_s} M_s R_{ox} \equiv A_{so} M_s \quad (6)$$

where M_s is the soot mass; ρ_s is the soot density; D_s is the soot particle diameter; MW_c is the molecular weight of carbon. R_{ox} is given by

$$R_{ox} = \left(\frac{K_A p_{O_2}}{1 + K_Z p_{O_2}} \right) x + K_B p_{O_2} (1 - x) \quad (7)$$

with

$$x = \frac{P_{O_2}}{P_{O_2} + K_T / K_B}$$

P_{O_2} is the partial pressure of oxygen. The model parameters are:

$$K_A = 20.0 \exp\left(-\frac{30000.0}{RT}\right);$$

$$K_B = 4.46 \times 10^{-3} \exp\left(-\frac{15200.0}{RT}\right);$$

$$K_T = 1.51 \times 10^5 \exp\left(-\frac{97000.0}{RT}\right);$$

$$K_Z = 21.3 \exp\left(-\frac{4100.0}{RT}\right),$$

where $R = 1.98 \text{ kcal/mol/K}$ [21]. Assuming that the transient changes in the oxygen and acetylene concentrations are negligible, the change of soot mass during one time step in a computational cell can thus be estimated as

$$\Delta M_s = \left(\frac{\dot{M}_{sf}}{A_{so}} - M_s \right) [1 - \exp(-A_{so} \cdot \Delta t)] \quad (8)$$

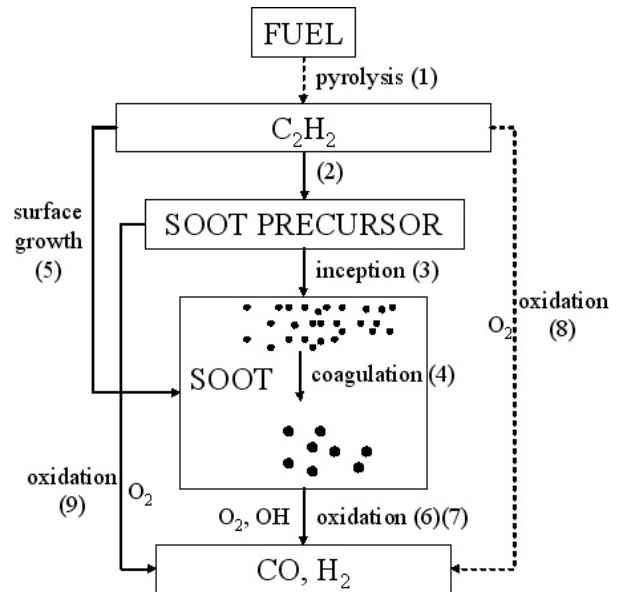


Figure 3. schematic of nine-step phenomenological soot model.

With the nine-step phenomenological soot model proposed by Tao et al. [13], the processes of soot formation and consumption are more detailed. Acetylene is viewed as the growth species. As illustrated in Fig. 3, the formation of acetylene is considered through fuel pyrolysis (Reaction 1). Acetylene is converted into a soot precursor (Reaction 2), or is oxidized by oxygen to form CO and H₂ (Reaction 8). The soot precursors are assumed to be C₆₀ in the present paper. After the initial soot particles are formed from soot precursors (Reaction 3), particle coagulation is considered (Reaction 4). Surface growth reaction via acetylene attack is considered using a hydrogen-abstraction/carbon-addition (HACA) mechanism (Reaction 5). Soot particles are oxidized via oxygen or OH attack (Reaction 6, 7). Reaction 9 is the oxidation of soot precursors by oxygen. The pyrolysis reaction (Reaction 1) and oxidation of acetylene (Reaction 8), which are indicated by dashed lines are included in the ERC reduced n-heptane mechanism. Therefore, these two reactions are not included in the soot model. The concentration of OH is also determined from CHEMKIN or from chemical equilibrium calculations, instead of estimating from the

quasi-steady state of the H_2 - O_2 - CO_2 reaction system as assumed by Tao et al. [13].

The net rate of soot mass fraction, Y_s and soot number density, N can be written as

$$\frac{dY_s}{dt} = MW_C (\dot{R}_3 + \dot{R}_5 - \dot{R}_6 - \dot{R}_7) \quad (9)$$

$$\frac{dN}{dt} = N_A \frac{MW_C}{MW_{nuc}} (\dot{R}_3 - \dot{R}_4) \quad (10)$$

where N_A is Avagadro's number and MW_{nuc} is the molecular weight of a particle nucleus. $\dot{R}_i$ is the reaction rate of the i -th reaction.

NUMERICAL RESULTS

VALIDATION OF KIVA-CHEMKIN AND GAMUT COMBUSTION MODELS

The combustion models were validated on the optically accessible HSDI engine. The engine was operated at 25% EGR rate, part-load (3 bar IMEP and 5 bar IMEP), and split-injection conditions. Two injection pressure cases, 800 bar and 1000 bar, were studied (for the 5 bar IMEP case, the injection pressures were 810 bar and 1010 bar). A 60° sector mesh of the HSDI engine, which is illustrated in Fig. 4, was used in the simulations. There are 30448, 13940, 10285 nodes at BDC, SOI (when chemistry starts to be calculated), and TDC, respectively. The numerical results obtained with the GAMUT combustion model were compared with experimental data and results from the KIVA-CHEMKIN model.

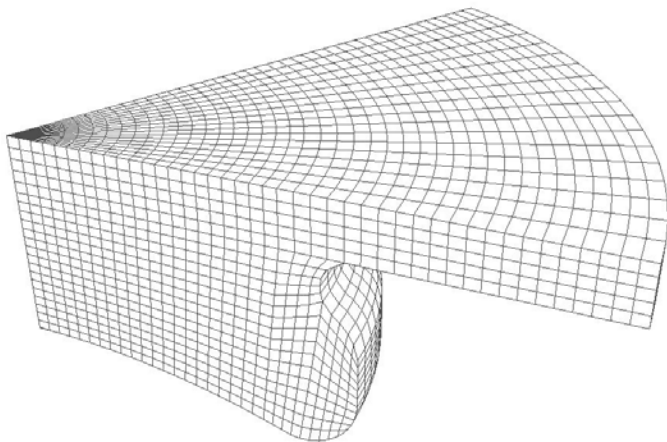


Figure 4. Perspective view of the 60° sector engine mesh.

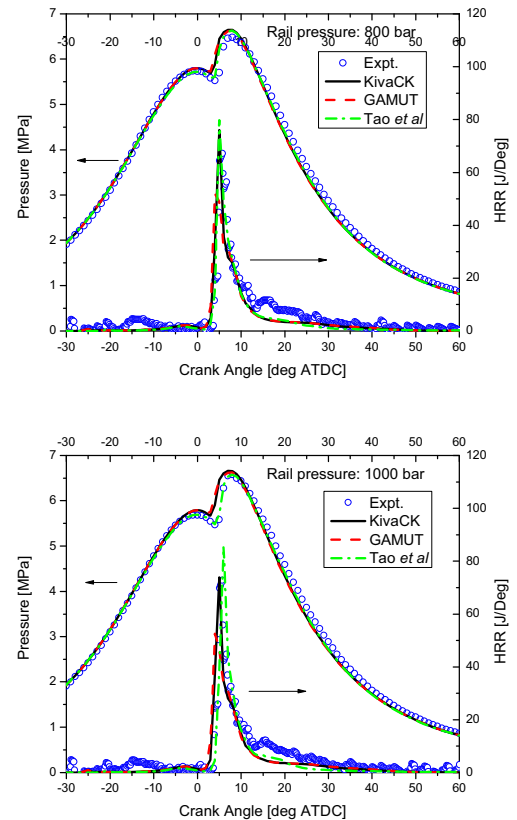


Figure 5. Pressure and heat release rate, IMEP= 3bar.

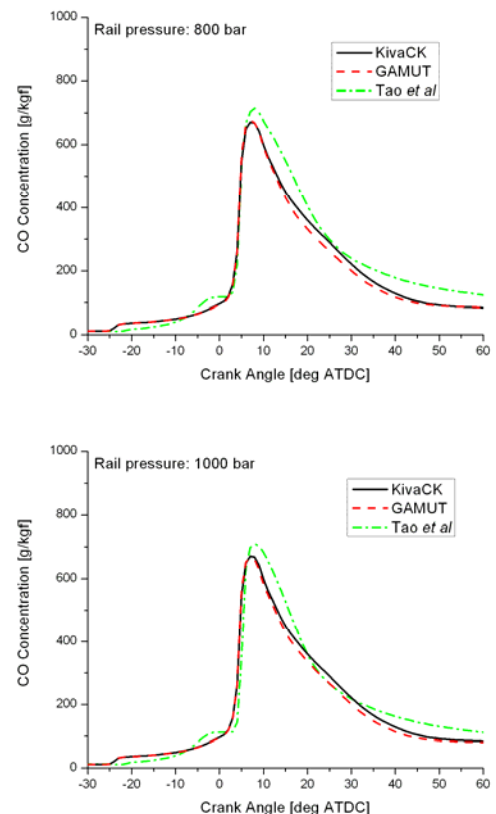


Figure 6. CO emissions, IMEP=3 bar.

Figure 5 shows in-cylinder pressure and heat release rates of the light-load case IMEP=3bar. Both the KIVA-CHEMKIN (solid line) and GAMUT (dashed line) models have very good agreement with the experimental data. Tao *et al.* [22] used the same KIVA-CHEMKIN code, mesh, and inputs, but a different chemical reaction mechanism. A much more comprehensive mechanism with 74 species and 338 elementary reactions was used. However, the current numerical results rival Tao's results, but only used about 34hr CPU time for each case compared to 1400hr in Tao's computations. The CO emissions of the three simulations are illustrated in Fig. 6. The present method gives very close profiles of CO to those of Tao's simulations, which implies that the present ERC reduced n-heptane mechanism is reliable, and very efficient. The results of the KIVA-CHEMKIN and GAMUT combustion models are very similar.

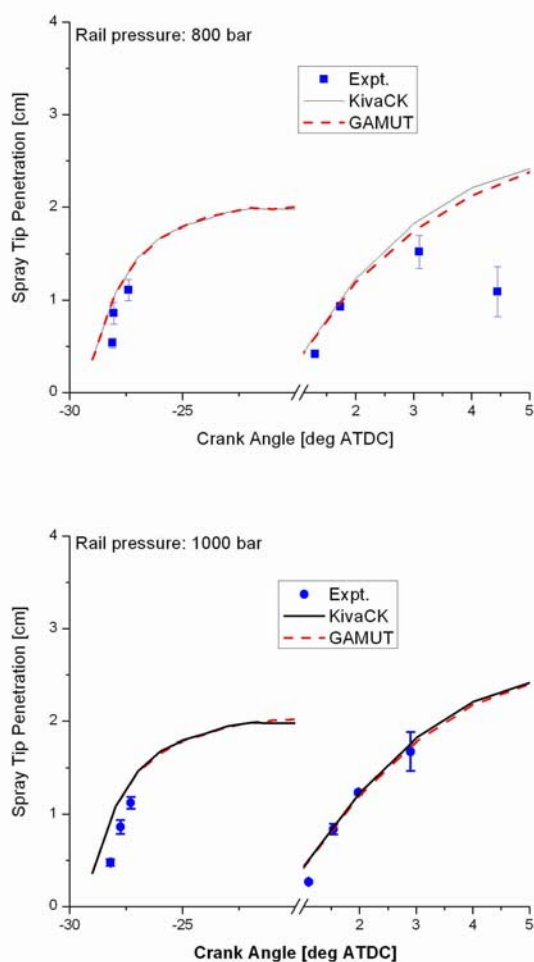


Figure 7. Spray penetration, IMEP=3bar.

Figure 7 shows profiles of spray tip penetration. The solid lines and dashed lines are the simulated results of the IMEP=3bar case using KIVA-CHEMKIN and GAMUT, respectively. Symbols are the measured spray tip penetration of the same nozzle in an engine-like, optically-accessible, high-pressure, constant-volume chamber. The chamber has a tunable swirl and

turbulence generator, as well as a piston bowl. Pilot injection was emulated. 0.8 mm^3 fuel was injected during the pilot injection and 8.0 mm^3 was injected during the main injection. The averaged experimental data and the corresponding error bars are evaluated from the measurements of the 6 spray plumes. The spray tip penetration mainly depends on the injection pressure, and the surrounding gas-phase environment. Before the pilot injection, there is no combustion and the properties of the gas (temperature and density) are very homogeneous. Therefore, the penetrations of different spray plumes are very close, i.e., the variances are small. In this stage, the KIVA-CHEMKIN and GAMUT combustion models give almost identical results, because the in-cylinder temperature is still below the critical temperature and no G-surface is initialized (i.e., the GAMUT combustion model has not started). The fuel was ignited about 2~3 degrees after the start of the main injection and the gas temperature and density becomes very inhomogeneous. The variances of the spray tip penetration then become larger because of the interaction between the droplets and the surrounding gas flow, including turbulent dispersion, inter-phase heat and mass transfer. In this stage, the KIVA-CHEMKIN

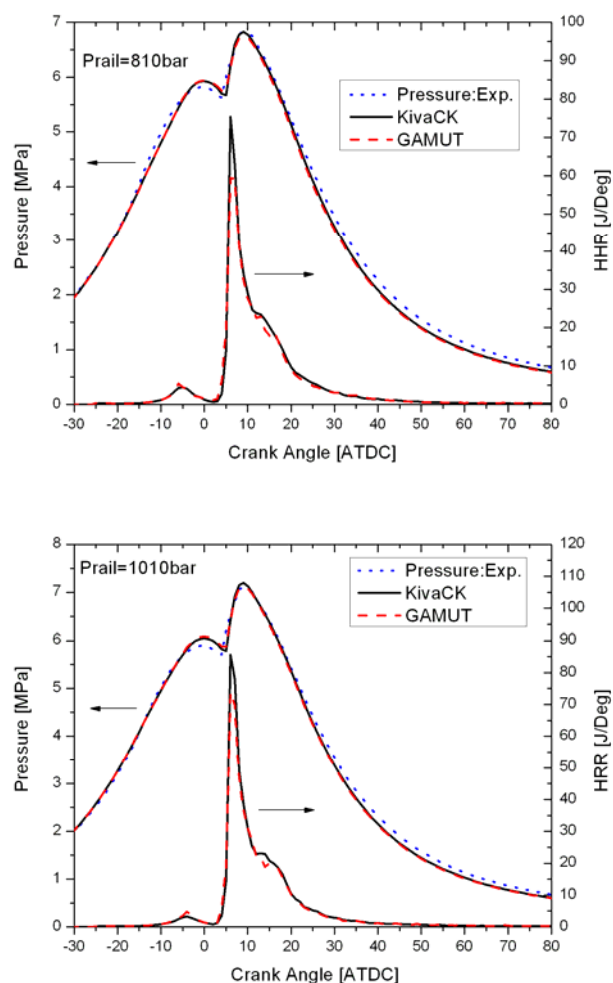


Figure 8. Pressure and heat release rate, IMEP=5bar.